netlognews

NETL's Quarterly R&D newsletter — October 2013, Issue 31

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U.S. DEPARTMENT OF ENERGY | the ENERGY lab NATIONAL ENERGY TECHNOLOGY LABORATORY

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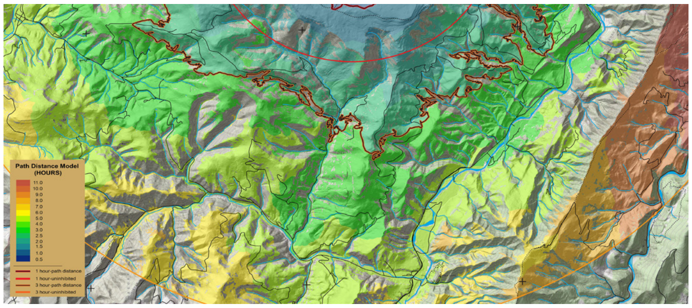
Cover image: Dr. Don Ferguson created a Path Distance Analysis model to help search and rescue teams find lost people that incorporates the potential time versus distance traveled by including impediments to foot traffic such as rivers, steep slopes, etc.

netlognews

newlognews is a quarterly newsletter highlighting recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.



Dr. Don Ferguson working on a computer model for search and rescue.

NETL Engineer's GIS Model Sought Nationwide for Life-Saving Search and Rescue

—Dr. Don Ferguson, a mechanical engineer in NETL's Thermal Science Division within the Office of Research and Development, has developed the Integrated Geospatial Tools for Search and Rescue, a suite of computational tools that uses Geographical Information Systems (GIS) applications to manage search and rescue operations for missing persons. These tools incorporate documented patterns of lost persons, related historical data, geographical data, and models, among a host of other criteria, to map out likely and/or probable locations of missing or lost persons.

In 2006, Dr. Ferguson's work with a local volunteer search and rescue group (Mountaineer Area Rescue Group) was awarded a grant from the U.S. Department of Homeland Security (DHS). This funding prompted the development of Dr. Ferguson's "lost-person incident model," a model based on the belief that a critical analysis of the geospatial environment, coupled with knowledge of lost-person behavior, translates to an understanding of how lost people might interact with the surrounding environment of vegetation, hills, streams, trails, roads, and various other geographic features. Dr. Ferguson also recognized that remote sensing and spatial data existed nationwide and could therefore be used to reduce and prioritize search areas to ultimately locate lost people much more quickly.

Understanding lost person behavior and how a person may interact with his environment is essential in developing strategies for quickly locating someone who is lost.

Dr. Ferguson's model and his vast experience with and knowledge of GIS have been successfully applied by several organizations, including the Department of Homeland Security, the Federal Bureau of Investigation, and the U.S. Department of Defense, to life-saving search and rescue operations.

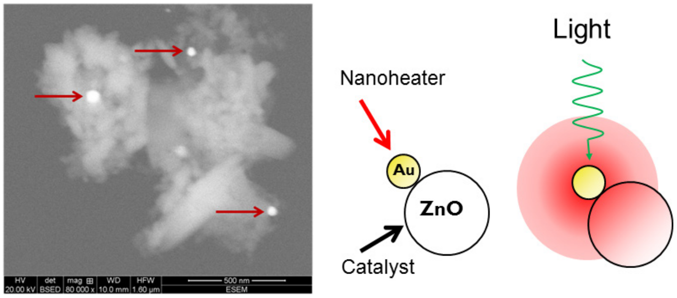
Contact: Donald Ferguson, 304-285-4192

geoWELL Provides Quick Access to Subsurface Geologic and Wellbore Websites

—Many NETL research portfolios rely on access to reliable information about subsurface engineering and natural systems data. In a combined effort with the Groundwater Protection Council, and with support from URS, Matrix Solutions, Coordinate Solutions, and Sextant Technical Services, NETL has created the GEO Water Energy Link Library, geoWELL, a map-based application that provides quick access to primary online sources of subsurface geologic and wellbore (oil, gas, and underground injection) information for appropriate U.S. state, tribal, and federal agencies. At the geoWELL site, users can access related federal agency links by selecting the 'United States Agencies' button.

On the site's interactive map, clicking on individual states populates a list of state- and tribal-specific links associated with subsurface geologic and wellbore information. The geoWELL application will assist NETL researchers and analysts as they seek information about these systems to support ongoing and future studies related to risks, impacts, and resources associated with fossil energy R&D. The geoWELL application is an Energy Data Exchange (EDX) tool. EDX is an online coordination and collaboration platform that supports energy research tech transfer and data needs. To learn more about geoWELL and other EDX tools, check out the September edition of NETL LabNotes and visit the EDX tools library.

Contact: Kelly Rose, 541-967-5883



Electron micrograph showing nanometer-sized plasmonic heaters (red arrows) dispersed on a zinc oxide catalyst material. This system is also shown schematically to the right of the micrograph.

Nanometer-Sized Plasmonic Heaters Convert Visible Light into Thermal Energy

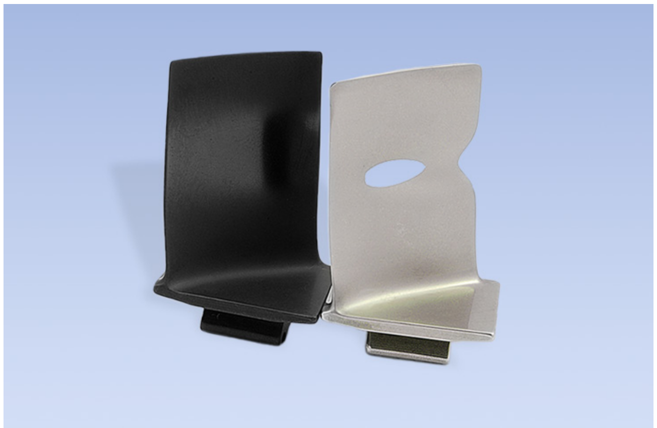
—A research team from NETL and West Virginia University has developed a new material capable of converting visible light into thermal energy, which can be used to drive the catalytic transformation of CO_2 to methane, carbon monoxide, and other light gases. These materials rely on a unique heating mechanism where light resonantly excites the collective motion of electrons, called plasmons, in nanometer-sized metal particles. These excited electrons dissipate their energy by colliding with the crystal lattice of the nanoparticles, generating heat in a process comparable to the ohmic heating that occurs when electrical currents are run through conducting metals.

The team has developed several catalyst systems that rely on using nanoparticulate gold (Au) and other materials as the optically active plasmonic heater and ZnO as the catalytically active substrate. Experimental results show that low-intensity visible light, comparable to what is achieved with standard solar concentrators, can heat the Au-ZnO catalysts up to ~600 °C in a controlled fashion, with product selectivity being dictated by light intensity. The results are described in an article appearing in the international journal, *Nanoscale*, published by the Royal Society of Chemistry (Nanoscale, 5, 6968, (2013), DOI: 10.1039/c3nr02001k). A U.S. provisional patent has also been filed on this technology.

Contacts: Christopher Matranga, 412-386-4114, Congjun Wang, 412-386-5815

NETL Wins Two 2013 R&D 100 Awards

Technologies developed by NETL researchers, in collaborative research efforts, have been recognized by R&D Magazine as two of the 100 most technologically significant products to enter the marketplace in the past year. The annual awards, known as the "Oscars of Invention," are selected by an independent panel of judges and the editors of R&D Magazine.



Comparison of a coated (left) versus an uncoated (right) rotor blade after a volcanic ash erosion test (image courtesy of MDS Coating Technologies Corporation).

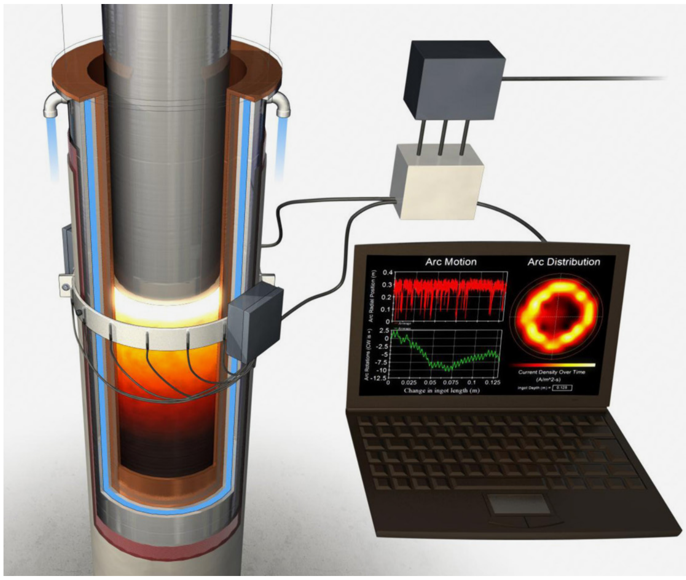
BlackGold® Coating Technology

An NETL-inspired partnership that combined MDS Coating Technology Corporation's **BlackGold®** coating innovation with the in-the-trenches knowledge of end users like Delta Airlines, and the materials performance expertise resident at NETL, has resulted in a new nanotechnology breakthrough in the marketplace.

During aircraft operation, gas turbine engines are continuously exposed to erosive media that are damaging to engine components. Nanostructured coatings applied to compressor airfoil surfaces can significantly reduce material loss leading to improved engine performance and fuel efficiency.

MDS Coating Technologies Corporation developed the composition of the **BlackGold®** coating technology. Delta Airlines evaluated this coating on high pressure compressor rotor blades in its engine fleet. Dr. Cynthia Powell and Dr. David Alman of the National Energy Technology Laboratory supported and contributed to this project by providing testing to optimize process variables and obtaining FAA certification. As a result of this collaboration, these three organizations helped bring this new nanocoating technology to market for airfoils in gas turbines.

The Federal Aviation Administration-approved nanocoating has the potential to save the U.S. commercial aviation industry up to 100 million gallons of fuel annually and cost savings greater than $300 million per year at today's jet fuel prices.

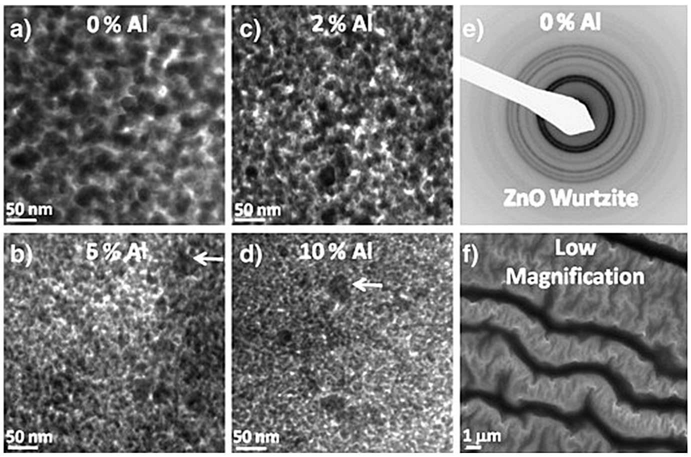


Set-up diagram for the Arc Position Sensing technology applied to a VAR furnace.

Arc Position Sensing Technology

Flaws in specialty metals used in aerospace and other advanced applications are often caused by solidification problems that arise during the melting and refining process. A common problem is arc constriction during melting.

The Arc Position Sensing (APS) technology, developed by NETL's Dr. Rigel Woodside and Dr. Paul King with support from Chris Nordlund at ATI Albany Operations, is a system that determines spatial locations of diffuse current segments (electric arcs) in real time. This allows operators to digitally monitor arc locations while melting and refining those metals—a technique that provides quality control critical for safety. For the first time ever, through use of the APS technology, precise measurements can be taken of the electric current conduction path within vacuum arc remelting (VAR) furnaces for industries that use specialty metals such as nickel, titanium, and zirconium. The technology may soon be used to help produce materials with stronger chemical and mechanical homogeneity, increasing the yield in the specialty metals and alloys used in the airline industry and in other advanced applications.



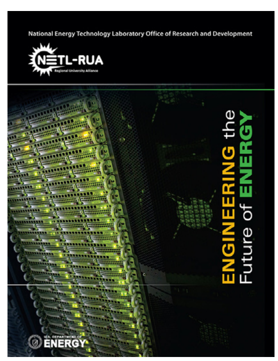
Transmission electron microscopy results obtained for selected Al-doped ZnO films prepared using the sol–gel technique including bright field images (a–d), a representative selected area diffraction pattern (e), and a low-magnification bright field image illustrating micron-scale film wrinkling (f).

High-Temperature Sensor Technologies to Increase Power Plant Efficiency

—The NETL sensors team is working on sensor technologies to enable embedded gas sensing at high temperature. The team's goal is to develop novel materials with large optical responses and high-temperature stability for integration with optical sensor platforms. High-temperature harsh environment conditions are relevant for a diverse range of advanced fossil energy applications, including solid oxide fuel cells, gas turbines, and advanced combustion systems. Real-time monitoring of critical process parameters could significantly impact existing power plants by increasing efficiency and reducing emissions. It would also encourage the successful adoption of next-generation fossil fuel-based power generation technologies. For high-temperature environments, optical sensor technologies offer benefits over alternative chemi-resistive gas sensors, which are limited by a need for electrical wiring to the embedded location and unstable electrical contacts and connections.

Through a combination of theoretical simulations and experiments, the team has demonstrated that transparent conducting oxides such as Al doped ZnO show significant promise for high-temperature optical gas sensing in the near infrared (IR) wavelength range. For this unique class of materials, electrical conductivity can be directly linked with the near IR optical absorption features, allowing for direct optical transduction of the more commonly investigated chemi-resistive sensing responses. In the case of nanoparticle-based films, a free electron resonance gives rise to a sharp absorption feature in the near-IR. To date, researchers have demonstrated useful sensing responses at temperatures approaching 700 °C using this approach. The team believes that higher temperatures are achievable in the future through the identification of transparent conducting oxide behavior in doped variants of higher temperature stable oxide systems. A recent article published in *Thin Solid Films*, 539 (2013) 327–336, discusses a demonstration of the concept for the Al-doped ZnO system. A non-provisional patent application on the concept was also filed on June 26, 2013 (U.S. 13,927,223).

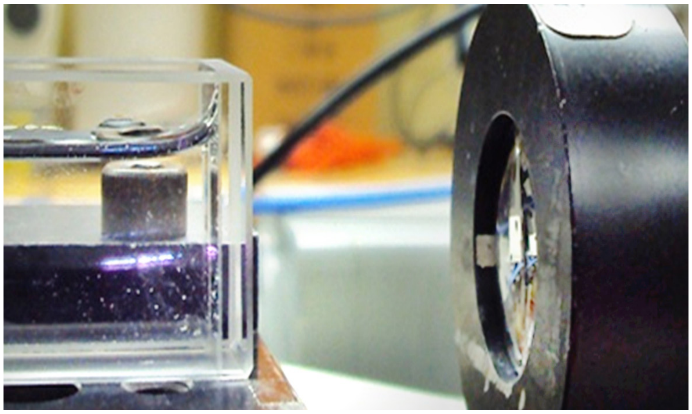
Contacts: Paul R. Ohodnicki, Jr. 412-386-7389, Congjun Wang, 412-386-5815, and Mark Andio, 412-386-4035



NETL-RUA Helps Engineer the Future of Energy

—Find out how the NETL-Regional University Alliance (NETL-RUA) teams lead research and educational initiatives to conceive and build a bridge to America's sustainable energy future.

Visit the e-book or download a print version of the brochure that describes how research can help fossil fuels contribute to short- and long-term energy solutions. From reducing our nation's CO_2 footprint to protecting human health and the environment to ensuring energy security, the goals of NETL and NETL-RUA are driving discoveries for clean, reliable, affordable energy supplies.



Laboratory laser spark production under water.

Compact, Portable Sensor Technology Monitors CO_2—

The availability of fossil fuels to provide clean, affordable energy is essential for domestic and global prosperity and security well into the 21st century. Carbon capture and storage in geologic formations is a promising technology to reduce the impact of CO_2 emissions on the environment. Monitoring capabilities that are reliable and cost effective are needed to confirm permanent storage of CO_2 in geologic formations. Improved monitoring technologies are needed for surface, near-surface, and subsurface applications to ensure that injection, abandoned, and monitoring wells are structurally sound and that CO_2 will remain within the injection formation.

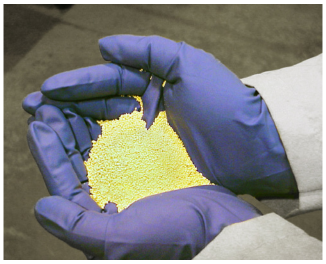
A team of researchers—Dr. Jinesh Jain (URS), Dr. Dustin McIntyre (NETL), and Dr. Steve Woodruff (NETL)—are studying laser-induced breakdown spectroscopy (LIBS) technology. The team developed a LIBS-based optical sensor for CO_2 leak monitoring and carbon sequestration research. The LIBS sensor employs a low peak power pumping pulse delivered by optical fiber to a laser, and the output can be used for field, underground, or underwater monitoring of carbon dioxide leaks. According to Drs. Jain and McIntyre, the availability of double pulsed laser systems and miniaturization components creates the potential to provide a compact, portable system for carbon sequestration field applications and Marcellus Shale research. The team has applied for a patent for this technology titled "A method and device for remotely monitoring an area using a low peak power optical pump."

Contact: Dustin McIntyre, 304-285-1374, Steven Woodruff, 304-285-4175

Robert Stevens (left) and Ranjani Siriwardane have developed a post-combustion method of capturing CO_2 from gas streams such as those from coal gasification.

Capturing CO_2 Using Magnesium Hydroxide Sorbent—

A new process based on a magnesium hydroxide ($Mg(OH)_2$) sorbent has been developed at NETL for CO_2 separation from warm-temperature (i.e., 150-250 °C) and high-pressure (i.e., > 380 psi) gas streams, such as coal gasification product streams. The process is described in a recently issued patent, U.S. patent 8,470,276. With this method, sorption of CO_2 takes place via formation of magnesium carbonate ($MgCO_3$), a white solid, that is then regenerated by decomposition at temperatures above 350 °C and re-hydroxylated with steam.



$Mg(OH)_2$, which can effectively capture CO_2 from warm-temperature, high-pressure gas streams and be regenerated for re-use.

CO_2 capture can be conducted as a post-combustion or pre-combustion process, but with either the challenge is to capture CO_2 in a way that minimizes energy penalty and cost. In both post-combustion and pre-combustion CO_2 capture scenarios, trace impurities such as sulfur dioxide, nitrogen oxides, and particulate matter in the CO_2-laden gas streams can degrade sorbents and reduce the effectiveness of certain CO_2 capture processes. The pre-combustion capture scenario features gas streams at elevated temperatures—other current technologies require cooling the gas stream prior to capture, which reduces the efficiency of an integrated gasification combined cycle (IGCC) power plant. Using $Mg(OH)_2$ for CO_2 in a post-combustion capture resolves some of these challenges.

The CO_2 removal process with $Mg(OH)_2$ is more favorable at high pressure, which makes it suitable for CO_2 removal downstream of the water-gas shift reactor in an IGCC system.

The process also works well in the presence of steam. Current commercial solvent-based processes require energy-intensive drying methods to remove moisture prior to CO_2 removal. Since the regeneration of the $Mg(OH)_2$ can be performed at high pressure in the presence of CO_2, the novel process significantly reduces the energy required for compression of CO_2, thereby increasing overall power plant efficiency.

Contact: Ranjani Siriwardane, 304-285-4513, Robert Stevens, 304-285-4305

NETL's mobile air monitoring laboratory

NETL and Maryland Department of the Environment Sign MOU—Many NETL research portfolios rely on access to reliable info In anticipation of lifting the current shale gas drilling moratorium in Maryland, the MDE requires an assessment of pre-development air quality so that comparisons can be made post-development to evaluate the impact of natural gas exploration and production activities on local air quality. A new memorandum of understanding between NETL and the MDE will enable the collection of baseline air quality data in Garrett and/or Allegheny Counties. Over the next two years, NETL will use its Mobile Air Monitoring Laboratory to conduct month-long monitoring in each of the four seasons. The laboratory trailer houses instruments designed to measure concentrations of criteria pollutants such as ozone, NO_2, PM_{10}, and $PM_{2.5}$; greenhouse gases such as methane and carbon dioxide; hazardous air pollutants and other non-methane volatile organic compounds; and a meteorological station to measure meteorological parameters. NETL plans to return to the area for post-development monitoring in future years to evaluate the activity's air quality impact.

Contact: Natalie Pekney, 412-386-5953

Computational Modeling on Sorbents Advances CO_2 Capture Technology—Researchers at NETL and their collaborators from the NETL-Regional University Alliance and the National University of Mexico have combined their expertise in computational modeling with experimental measurements to conduct a comprehensive study on the CO_2 capture properties of mixtures of Li_2O/SiO_2 and Li_2O/ZrO_2 solids. The scientists examined the calculated thermodynamic and measured kinetic properties of mixtures with various ratios of Li_2O to SiO_2 and Li_2O to ZrO_2 Results of the experiments indicated that a higher concentration of SiO_2 or ZrO_2 in a mixture increased the ability of the mixture to withstand heat, making it a feasible candidate for use in carbon capture applications in the extreme temperature environments of a power plant. Current commercial CO_2 capture technology is expensive and energy intensive, and research into developing materials that will reduce costs and improve efficacy is vital.

Individual sorbents may not meet the requirements necessary for successful industry application, however, this study demonstrated that by mixing or doping two or more materials to create a new material, it is possible to move the temperature window of sorbent capture-release CO_2 into the range of desired operating conditions. This method provides a way to synthesize new sorbents engineered for optimal performance.

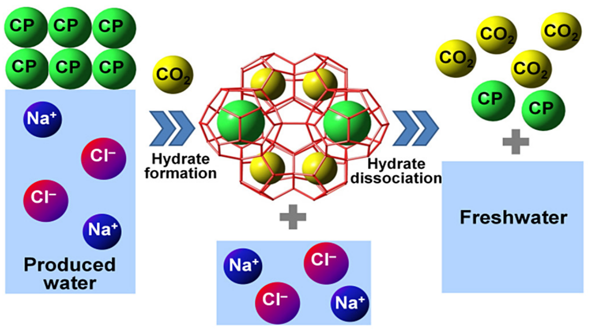
The results of this study have appeared in two articles in the Royal Society of Chemistry's international journal *Physical Chemistry Chemical Physics*. The articles summarized the current progress of research on lithium-based solid sorbents and described three mixing scenarios to provide illumination and general guidelines on the process of designing new CO_2 sorbents. Additionally, the work was presented at the 2013 ACS Spring Meeting, and 12th International Conference on Carbon Dioxide Utilization.

Contact: Yuhua Duan, 412-386-5771

New Method Developed for Producing Potable Water Using Gas Hydrates

Hydrates—As the shale gas boom continues, NETL scientists are finding an economical way to turn the briny wastewater produced during hydraulic fracturing and other oil and gas extraction processes into water suitable for drinking and irrigation.

The innovative desalination process removes 90 percent of the salt from wastewater. Oil and gas extraction methods produce almost 10 barrels of extremely salty water per barrel of oil. In arid regions, that water could be a valuable resource; however, traditional desalination methods are costly and energy intensive. NETL's new method uses two hydrate formers, taking advantage of their potential to elevate gas hydrate formation temperatures and kinetics. The method can subsequently increase the energy efficiency of the gas hydrate desalination process, particularly for treating high salinity produced water. When gas hydrates form in produced wastewater, the hydrate consists of only water and natural gas, leaving behind salts and other impurities.

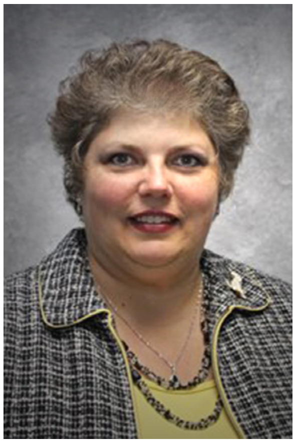


NETL's new gas hydrate-based desalination process uses water-immiscible hydrate formers—cyclopentane (CP) and cyclohexane (CH)—as secondary hydrate guests to alleviate temperature requirements for hydrate formation.

When gas hydrates break down, they release only gas and pure water. Traditional methods for using gas hydrates to desalinate water were not economically feasible because water must be chilled to 28 degrees Fahrenheit in order for gas hydrates to form. NETL researchers sought a hydrate former that can elevate the hydrate formation temperature and eliminate the cost of chilling. They discovered that cyclopentane and cyclohexane hydrates along with CO_2 molecules could form gas hydrates at higher, near-room temperatures to desalinate produced water with high salinity. An additional benefit: the desalinated water can be easily separated due to the water immiscibility of cyclopentane and cyclohexane.

The development and laboratory testing of this new gas hydrate desalination technique is described in the ACS journal *Sustainable Chemistry & Engineering*.

Contact: Yongkoo Seol, 304-285-2029,
Jong-Ho Cha, 304-285-0937



The Pittsburgh Federal Executive Board selected Lisa Soukup as its 2013 Woman of the Year. Ms. Soukup's own career has spanned finance, communications, and information technology.

NETL Champion for Women Takes the Gold—Lilas Soukup, an employee of NETL for 35 years, was recently recognized by the Pittsburgh Federal Executive Board as its 2013 Woman of the Year.

The Board cited in particular Ms. Soukup's leadership of the NETL Federal Women's Program. In this role, she works with the Labor Management Partnership Council and the American Federation of Government Employees to expand the part women play throughout the laboratory. When this partnership began 15 years ago, advancement of female employees at NETL was achieved almost exclusively through administrative and other staff positions. Today, women head operational and research divisions, manage multimillion dollar technology-development projects, and lead cutting edge research teams.

To directly support the effort, Ms. Soukup acts as a mentor with the Department of Energy's (DOE) Mickey Leland Energy Fellowship, a summer internship program that provides hands-on work experience to female and minority students pursuing degrees in STEM majors. She is also an active member of the DOE Energy Council on Women and Girls— a branch of the White House Council on Women and Girls— which seeks to increase women's participation in America's STEM workforce and economy.

In addition, Ms. Soukup champions NETL's educational outreach to elementary, middle school, and high school students. She is the long-time lead organizer for the Southwestern Pennsylvania Science Bowl, an annual science and math competition sponsored by the laboratory to select teams for DOE's National Science Bowl. She also holds a position on the National Science Bowl Committee, which oversees the competition held each spring in Washington, D.C.

Ms. Soukup was surprised and honored by the recognition of the Pittsburgh Federal Executive Board. "In the past few years, I have watched young women here achieve more than previous generations of women could have dreamed," she said. "And I am proud to have been a part of such a positive change at NETL."

NETL Researcher Named AIChe Fellow—Dr. Madhava Syamlal, NETL Computational and Basic Sciences Focus Area Lead, recently was named a Fellow of the American Institute of Chemical Engineers. Dr. Syamlal has been a member of AIChE since 1983, and a Senior Member since 1987.

AIChE Fellows are recognized for their professional attainment and significant accomplishments in engineering. They are nominated and recommended by various Fellows and Senior Members within AIChE. Dr. Syamlal joins a distinguished group of more than 800 members from around the globe.

Dr. Syamlal is currently involved with several projects, including NETL-Regional University Alliance's Multiphase Flow with Interphase eXchanges (MFIX) and the Carbon Capture Simulation Initiative research teams.

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Patents Issued This Quarter

1.	Method for Designing a Reforming and/or Combustion Catalyst System. David A. Berry (NETL), Dushyant Shekhawat (NETL); Mark Smith (REM Engineering); Daniel Haynes (URS); **8,486,301**, issued July 16, 2013.
2.	Regenerable Sorbent Technique for Capturing CO_2 Using Basic Immovilized Amine Sorbents. Henry W. Pennline; James. S. Hoffman; Daniel J. Fauth; McMahan L. Gray; and Kevin P. Resnick; **8,500,854**, issued August 6, 2013.
3.	Regenerable Solid Amine Sorbents, McMahan L. Gray (NETL); Daniel J. Fauth (NETL); Kenneth J. Champagne (NETL); Eric Beckman (University of Pittsburgh); **8,530,375**, issued September 10, 2013.

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